Statistical mixtures of states can be more quantum than their superpositions: Comparison of nonclassicality measures for single-qubit states

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A bosonic state is commonly considered nonclassical (or quantum) if its Glauber-Sudarshan P function is not a classical probability density, which implies that only coherent states and their statistical mixtures are classical. We quantify the nonclassicality of a single qubit, defined by the vacuum and single-photon states, by applying the following four well-known measures of nonclassicality: (1) the nonclassical depth, τ , related to the minimal amount of Gaussian noise which changes a nonpositive P function into a positive one; (2) the nonclassical distance D, defined as the Bures distance of a given state to the closest classical state, which is the vacuum for the single-qubit Hilbert space; together with (3) the negativity potential (NP) and (4) concurrence potential, which are the nonclassicality measures corresponding to the entanglement measures (i.e., the negativity and concurrence, respectively) for the state generated by mixing a single-qubit state with the vacuum on a balanced beam splitter. We show that complete statistical mixtures of the vacuum and single-photon states are the most nonclassical single-qubit states regarding the distance D for a fixed value of both the depth τ and NP in the whole range [0, 1] of their values, as well as the NP for a given value of τ such that $\tau > 0.3154$. Conversely, pure states are the most nonclassical single-qubit states with respect to τ for a given D, NP versus D, and τ versus NP. We also show the "relativity" of these nonclassicality measures by comparing pairs of single-qubit states: if a state is less nonclassical than another state according to some measure then it might be more nonclassical according to another measure. Moreover, we find that the concurrence potential is equal to the nonclassical distance for single-qubit states. This implies an operational interpretation of the nonclassical distance as the potential for the entanglement of formation.

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I. INTRODUCTION

One of the central problems of quantum theory, already raised by its founders [1–4], is the question of testing whether a given physical system cannot be properly described classically. This problem has attracted special interest in quantum optics [5, 6], quantum information [7, 8], and recently even in quantum biology [9, 10]. In this paper, we address the problem of not only testing but also quantifying nonclassicality (or quantumness) of light or, more generally, of a bosonic system.

In general, a state is referred to as *nonclassical* if its Glauber-Sudarshan P function [11, 12] cannot be considered a classical probability density [13], which means that it is not positive (semidefinite). In other words, a state that cannot be expressed as a statistical mixture of coherent states is called nonclassical. Otherwise the state is considered classical. It is worth noting that if the P function is more singular than the Dirac δ -function (which is the case for, e.g., the Fock states), then it is also nonpositive. Thus, the nonpositivity of the P function is the necessary and sufficient condition for nonclassicality.

There exist several criteria of nonclassicality. However, most of these criteria can only show a signature of nonclassicality. They do not provide any quantitative measure of the nonclassicality. Thus, they cannot be used to compare the

amount of nonclassicality present in two different states. Besides the above-mentioned P-function-based criterion of nonclassicality, all the finite sets of other criteria are sufficient but not necessary. Only an infinite set (or hierarchy) of nonclassicality criteria can be considered a sufficient and necessary condition of nonclassicality (see, e.g., Ref. [14]). Thus, these finite-set criteria of nonclassicality may be better viewed as witnesses of nonclassicality rather than measures of nonclassicality. This limitation of the existing criteria of nonclassicality is well known and several efforts have been made to quantify nonclassicality. These efforts led to the introduction of various measures of nonclassicality.

For example, in 1987, Hillery introduced a distance-based measure of nonclassicality [15]. Specifically, the trace distance of a quantum state from the nearest classical state can be considered as a measure of nonclassicality associated with the given quantum state. This idea of distance-based measures has attracted considerable attention in quantum optics [16–20]. This intuitive definition is easy to understand but extremely difficult to compute as it requires minimization over an infinite number of variables. Specifically, one needs to minimize over the set of all possible classical states in order to identify an optimal reference classical state that yields a minimum distance with respect to a given nonclassical state. This is the main problem associated with the distance-based mea-

sures of nonclassicality. Because of this computational difficulty, until now the nonclassical distance has not exactly been computed for any nonclassical state according to the original definition. However, the computational difficulty associated with Hillery's original measure can be circumvented by measuring the distance of a given nonclassical state from a specific class of classical states. This approach was adopted in a few works. For example, Marian et al. [18] defined a simplified version of the Hillery nonclassical distance for a single-mode Gaussian state of a radiation field as the Bures distance between the state and the set of all classical single-mode Gaussian states. Wünsche et al. [16, 17] measured the distance of a given state from the set of only coherent states. Specifically, they used the Hilbert-Schmidt distance of a pure state ρ from the coherent states as a quantitative measure of nonclassicality of ρ [17]. Almost in the similar line, Mari et al. [21] introduced a measure of nonclassicality of a state ρ in terms of its trace-norm distance from the set of all states having the positive Wigner function. Strictly, speaking this quantifier of nonclassicality is not a proper measure since some nonclassical states do have positive Wigner function (as discussed below with respect to a nonclassicality volume). Similarly, Dodonov and Renó [20] used the Hilbert-Schmidt distance from the set of all displaced thermal states as a quantitative measure of nonclassicality. These measures are naturally free from the problem that arises due to the minimization over the set of arbitrary classical states.

In 1991, Lee [22] introduced a quantitative measure of nonclassicality which is usually referred to as nonclassical depth. It is well known that noise can destroy nonclassicality. Lee used this property to define the nonclassical depth as the minimum amount of noise required to destroy the nonclassicality. This measure is not continuous and for every non-Gaussian pure state it is always equal to 1 [23]. As a consequence, one cannot use this measure to compare the amount of nonclassicality present in two non-Gaussian pure states. The nonclassical depth was applied in dozens of papers (see, e.g., Refs. [23– 25] and for reviews see Refs. [5, 26]).

In 2004, Kenfack and Życzkowski [27] introduced the concept of the nonclassical volume, which is a quantitative parameter of nonclassicality corresponding to the volume of the negative part of the Wigner function. A non-zero value of the volume definitely indicates the existence of nonclassical state, but this volume is not useful as a measure in general, since the Wigner function cannot detect the presence of nonclassicality in all quantum states. Specifically, the Wigner function of a squeezed coherent state is not negative. As a consequence, the nonclassical volume vanishes for all squeezed coherent states, although they are nonclassical according to the definition based on the nonpositivity of the *P* function. This example implies that, in general, the nonclassical volume is not an appropriate measure of nonclassicality.

Various other methods to test (or witness) nonclassicality (see, Ref. [13] and references therein) and quantify it [28–30] have been developed by Vogel *et al.* In particular, the nonclassicality witnesses [14], based on the matrices of the normally-ordered moments of, e.g., annihilation and creation operators, have attracted considerable interest as an infinite set of

observable conditions corresponding to a necessary and sufficient condition for nonclassicality. Various generalizations have been studied, including tests of spatiotemporal nonclassical properties of multimode fields [31–33]. Moreover, this approach was the inspiration to introduce entanglement witnesses based on the matrices of moments of annihilation and creation operators of the partially-transposed density matrices [34, 35] (for generalizations see, e.g., Refs. [36, 37]). The relations between these entanglement and nonclassicality criteria were also studied in detail (see, e.g., Ref. [32]). Note that the majority of these works have solely described nonclassicality (or entanglement) witnesses rather than nonclassicality measures. Only the more recent works of Vogel et al. (see, e.g., Refs. [28-30]) were focused on quantifying nonclassicality. For example, an experimentally-accessible method to determine a degree of nonclassicality was recently described in Ref. [30].

With the advances in quantum computation and information, many measures of entanglement (which is a specific manifestation of nonclassicality) have been studied. Unfortunately, measures of entanglement cannot be applied directly to all nonclassical states. For example, nonclassicality of single-mode states cannot be measured directly by using a measure of entanglement. Interestingly, an indirect way to use measures of entanglement as measures of nonclassicality was suggested by Asboth et al. [38]. Specifically, if a singlemode nonclassical (classical) state is combined with the vacuum at a beam splitter, then the output state will be entangled (separable), for which various entangled measures can be applied. For example, in the original Ref. [38], the relative entropy of entanglement and the logarithmic negativity (referred to as entanglement potentials) were applied as measures of entanglement produced at the output of a balanced beam splitter as the result of combining a nonclassical state with the vacuum. In principle, one can use any other measure of entanglement (e.g., the concurrence related to the entanglement of formation) to measure nonclassicality using this approach. Recently, Vogel and Sperling [29] studied the approach in Ref. [38] to measure nonclassicality based on the Schmidt rank as an entanglement potential. Note that this measure based on the Schmidt rank is discontinuous (analogously to the nonclassical depth, as it is explained in detail in Sec. III A). Here we apply the continuous entanglement potentials, which are based on the negativity and concurrence.

It is important to clarify our usage of the term *entangle-ment potential*, which is more general than that used in the original Refs. [29, 38]. Specifically, we use this notion by referring to any entanglement measure applied to the output of the auxiliary beam splitter used in Ref. [38]. Thus, in our understanding, the following measures can be considered as special cases of entanglement potentials: the negativity and concurrence potentials, as well as those based on (i) the logarithmic negativity, (ii) relative entropy of entanglement, and (iii) Schmidt numbers. However, strictly speaking, Asboth *et al.* [38] referred solely to the measure (i) as the entanglement potential, while to the measure (ii) as the entropic entanglement potential. Moreover, Vogel and Sperling [29] are not referring to the measure (iii) as an entanglement potential at

all.

We analyze the nonclassicality of states only. Note that the nonclassicality of operations (see, e.g., Refs. [39–41]) can also be studied by applying various measures.

The discussion above shows that there exists a large number of quantitative measures of nonclassicality. However, none of the measures can be considered as superior as all of them have some limitations and different physical (or operational) interpretations. Here we discuss the relativity of a set of nonclassicality measures which can be observed even for the simplest nontrivial case of a single qubit defined as a coherent or incoherent superposition of the vacuum and single-photon states. We also report our analytical solutions for the Lee nonclassical depth, the negativity potential, and the Hillery nonclassical distance. The latter is found to be equivalent to the concurrence potential. Further, we find boundary states, which are maximally nonclassical states according to one nonclassicality measure for a given value of another nonclassicality measure.

It is well known, and already confirmed experimentally [42], that statistical mixtures of the vacuum and single-photon states are nonclassical (except for the vacuum). We find, which is the most important result of this paper, that such statistical mixtures can be more nonclassical than coherent or partially incoherent superpositions of the vacuum and single-photon states. This can be noticed by comparing their nonclassicality for two chosen measures.

For the clarity of our presentation, we analyze the algebraically-simplest nonclassical states, i.e., single-qubit states, which can be written in a general form in the Fock basis as follows:

$$\rho(p,x) \equiv [\rho_{mn}] = \begin{bmatrix} 1-p & x \\ x^* & p \end{bmatrix}, \tag{1}$$

where the parameters are $p \in [0,1], |x| \in [0,\sqrt{p(1-p)}],$ and m,n=0,1.

The paper is organized as follows. In Sec. II, we recall the definitions of four popular nonclassicality measures. And, more importantly, we find analytical formulas for these measures for arbitrary single-qubit states. In Sec. III, we present the main results of this paper, which show the relativity of ordering states with respect to their degree of nonclassicality. We also demonstrate that the nonclassicality of mixed states can exceed that of superposition states. We conclude in Sec. IV.

II. NONCLASSICALITY MEASURES FOR SINGLE-QUBIT STATES

A. Nonclassical depth

Here recall the concept of the nonclassical depth τ introduced by Lee [22, 24] (for a review see Ref. [5] and references therein). We present the definition of τ in a slightly different form as based on the standard Cahill-Glauber s-parametrized quasiprobability distribution (QPD) rather than

the R-function used by Lee. Then we find a compact formula for the nonclassical depth for arbitrary single-qubit states.

We start from the Fock-state representation of the s-parametrized QPD, $W^{(s)}(\alpha)$, for an arbitrary-dimensional state ρ as [43]

$$W^{(s)}(\alpha) = \sum_{m,n=0}^{\infty} \rho_{mn} \langle n | T^{(s)}(\alpha) | m \rangle, \tag{2}$$

given in terms of

$$\langle n|T^{(s)}(\alpha)|m\rangle = c\sqrt{\frac{n!}{m!}}y^{m-n+1}z^n(\alpha^*)^{m-n}L_n^{m-n}(x_\alpha),$$
(3)

where $s\in[-1,1],\ c=\frac{1}{\pi}\exp[-2|\alpha|^2/(1-s)],\ x_\alpha=4|\alpha|^2/(1-s^2),\ y=2/(1-s),\ z=(s+1)/(s-1),\ \text{and}\ L_n^k(x_\alpha)$ are the associate Laguerre polynomials [44]. In special cases, $L_0^k(x_\alpha)=1$ and $L_1^k(x_\alpha)=1+k-x_\alpha$. Moreover, α is a complex number, where its real and imaginary parts can be interpreted as canonical position and momentum, respectively. The operator $T^{(s)}(\alpha)$ is defined in the Fock representation by Eq. (3) or, equivalently, by the formula $T^{(s)}(\alpha)=\frac{1}{\pi}yz^{(a^\dagger-\alpha^*)(a-\alpha)},$ where a (a^\dagger) is the annihilation (creation) operator. In the special cases of s=-1,0,1,1, the QPD $W^{(s)}(\alpha)$ becomes the Husimi Q, Wigner W, and Glauber-Sudarshan P functions, respectively.

For a general single-qubit state, Eq. (2) reduces to

$$W^{(s)}(\alpha) = cy[\rho_{00} + z(1 - x_{\alpha})\rho_{11} + 2y\text{Re}(\alpha\rho_{01})].$$
 (4)

As already explained, the standard definition of nonclassicality is based on the nonpositivity of the P function. The s-parametrized QPDs can be used to quantify the degree of nonclassicality. For example, the concept of the nonclassical depth of Lee [22] can be easily understood by recalling the relation between two QPDs, $\mathcal{W}^{(s_1)}$ and $\mathcal{W}^{(s_2)}$ with $s_2 < s_1$:

$$\mathcal{W}^{(s_2)}(\alpha) = c' \int \exp\left(-\frac{2|\alpha - \beta|^2}{s_1 - s_2}\right) \mathcal{W}^{(s_1)}(\beta) d^2\beta, \quad (5)$$

where $c'=2/[\pi(s_1-s_2)]$. It is seen that all the QPDs can be obtained from the P function $(s_1=1)$ by its convolution with the Gaussian noise. By decreasing the parameter s from 1, the P function for a given nonclassical state becomes nonnegative at some value (say s_0). This is because the Husimi function (s=-1) is non-negative for any state. The Lee nonclassical depth τ is simply related to this Cahill-Glauber parameter s_0 , viz. $\tau=(1-s_0)/2$.

From the QPD, given by Eq. (4), for a general single-qubit state, we can write that

$$\tau = \frac{1 - s_0}{2} = \frac{1}{2} - \frac{1}{2} \min_{\alpha} s_{-}(\alpha), \tag{6}$$

where

$$s_{-}(\alpha) = 1 + [2\operatorname{Re}(\alpha x) - p] - \sqrt{[2\operatorname{Re}(\alpha x) - p]^2 - 4p|\alpha|^2}.$$
(7)

We found analytically the minimum of Eq. (6), which leads to the following simple general formula for the nonclassical depth of an arbitrary single-qubit state, given in Eq. (1):

$$\tau[\rho(p,x)] = \frac{\rho_{11}^2}{\rho_{11} - |\rho_{01}|^2} = \frac{p^2}{p - |x|^2},\tag{8}$$

assuming $p \in (0,1]$ and $|x| \in [0,\sqrt{p(1-p)}]$. While for p=0, the formula is simply given by $\tau[\rho(0,0)]=0$.

B. Entanglement potentials

Here we study the negativity and concurrence potentials as measures of nonclassicality based on the unified description of nonclassicality and entanglement by applying a beam-splitter (BS) transformation as introduced in Ref. [38].

The BS transformation can formally be described by the Hamiltonian $H=\frac{1}{2}(a^{\dagger}b+ab^{\dagger})$, where $a=|0\rangle\langle 1|=[0,1;0,0]$ and, analogously, b are the annihilation operators of the input modes. The unitary transformation $U_{\rm BS}=\exp(-iHt)$ in the four-dimensional Hilbert space can be written as

$$U_{\rm BS} = \begin{bmatrix} 1 & 0 & 0 & 0\\ 0 & \cos(t/2) & -i\sin(t/2) & 0\\ 0 & -i\sin(t/2) & \cos(t/2) & 0\\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{9}$$

where, for simplicity, we set $\hbar=1$. In general, $T=\cos^2(t/2)$ and $R=\sin^2(t/2)$ correspond to the BS transmittance and reflectance, respectively. A balanced beam splitter (with T=R) corresponds to the evolution time $t=\pi/2$.

The state ρ_{out} , which is the output of the BS with a general single-qubit state ρ , given in Eq. (1), and the vacuum at the two input ports, is given by

$$\rho_{\text{out}} = U_{\text{BS}}(\rho \otimes |0\rangle\langle 0|)U_{\text{BS}}^{\dagger}.$$
 (10)

In the special case for the balanced BS we have

$$\rho_{\text{out}}(p,x) = \begin{bmatrix} 1-p & \frac{1}{\sqrt{2}}ix & \frac{1}{\sqrt{2}}x & 0\\ -\frac{1}{\sqrt{2}}ix^* & \frac{1}{2}p & -\frac{1}{2}ip & 0\\ \frac{1}{\sqrt{2}}x^* & \frac{1}{2}ip & \frac{1}{2}p & 0\\ 0 & 0 & 0 & 0 \end{bmatrix}.$$
(11)

The output state is entangled (except when the input is in the vacuum state) as can be verified by applying entanglement measures. Here we apply the negativity N and concurrence C for the BS output state $\rho_{\rm out}$, which can be interpreted as non-classicality measures referred to as entanglement potentials of an input state ρ .

1. Negativity potential

The negativity potential (NP) of a single-mode input state ρ can be defined as the negativity N of the two-mode output state $\rho_{\rm out}$, i.e.,

$$NP(\rho) \equiv N(\rho_{out}).$$
 (12)

Recall that the negativity for two qubits is given by [8]

$$N(\rho_{\text{out}}) = \max[0, -2\min\operatorname{eig}(\rho_{\text{out}}^{\Gamma})], \tag{13}$$

which is proportional to the negative eigenvalue of the matrix $\rho_{\rm out}^{\Gamma}$ corresponding to the partial transpose of $\rho_{\rm out}$ with respect to one of the qubits. Thus, it is seen that the negativity corresponds to the Peres-Horodecki separability condition based on the partial transpose [45, 46]. The negativity [or more precisely the logarithmic negativity, $\log_2(N+1)$] has an operational interpretation as the entanglement cost under operations preserving the positivity of partial transpose (PPT) [47, 48]. It was also shown that the number of entangled degrees of freedom of two subsystems can be estimated from the negativity [49]. Thus, in analogy to these interpretations, the NP can be also referred to as the entanglement potential for the estimation of entangled dimensions or the potential for the PPT entanglement cost.

We find that the NP for an arbitrary single-qubit state $\rho(p,x)$ can be given by the following formula:

$$NP[\rho(p,x)] = \frac{1}{3} \left[2Re \left(\sqrt[3]{2\sqrt{a_1} + 2a_2} \right) + p - 2 \right], \quad (14)$$

where

$$a_1 = a_2^2 - 2[5(p-1)p + 6|x|^2 + 2]^3,$$

 $a_2 = 14p^3 - 21p^2 + 15p + 9(p-2)|x|^2 - 4.$ (15)

This solution was found by solving the following equation for the negativity [50]:

$$48 \det \rho^{\Gamma} + 3N^4 + 6N^3 - 6N^2(\Pi_2 - 1)$$
$$-4N(3\Pi_2 - 2\Pi_3 - 1) = 0, (16)$$

which is given in terms of the measurable and invariant moments $\Pi_n=\mathrm{Tr}[(\rho^\Gamma)^n]$. The negativity is given by a much more complicated formula than those for any other nonclassicality measures studied here. Surprisingly, a direct calculation of the eigenvalues of $\rho_{\mathrm{out}}^\Gamma$ can result even in a more complicated formula. Of course, Eq. (14) can be considerably simplified in special cases. For example, the NP for $\rho'=\rho(p=1/8,x=1/4)$ reads

$$NP(\rho') = \frac{1}{4}\sqrt{26}\cos\left\{\frac{1}{3}\left[\pi - \arctan\left(\frac{1}{66}\sqrt{38}\right)\right]\right\} - \frac{5}{8}.$$
 (17)

The NP for other special states, which are important in our comparisons, are analyzed in Sec. III.

2. Concurrence potential

In analogy to the NP, the concurrence potential (CP) of a given single-qubit state ρ can be given in terms of the concurrence C of the two-qubit output state $\rho_{\rm out}$, viz.,

$$CP(\rho) \equiv C(\rho_{out}).$$
 (18)

The concurrence for a general two-qubit system is defined as [51]:

$$C(\rho_{\text{out}}) = \max \left\{ 0, 2 \max_{j} \lambda_{j} - \sum_{j} \lambda_{j} \right\}, \quad (19)$$

where $\{\lambda_j^2\} = \text{eig}[\rho_{\text{out}}(\sigma_2 \otimes \sigma_2)\rho_{\text{out}}^*(\sigma_2 \otimes \sigma_2)]$, and σ_2 is the Pauli operator. This measure is monotonically related to the entanglement of formation, E_F , as follows [51]:

$$E_F = h\left(\frac{1}{2}[1 + \sqrt{1 - C^2}]\right),$$
 (20)

which is given via the binary entropy $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$. Thus, the CP can also be referred to as the potential for the entanglement of formation. A direct calculation of the CP of $\rho(p,x)$ leads us to a particularly simple formula

$$CP[\rho(p,x)] = 1 - \langle 00|\rho_{out}|00\rangle = \rho_{11} = p,$$
 (21)

for $p \in [0, 1]$ and $|x| \in [0, \sqrt{p(1-p)}]$.

C. Nonclassical distance

Here we calculate the nonclassical distance D, which is the Hillery measure of nonclassicality (see, for a review, Ref. [5] and references therein) for a specifically chosen set of classical states. We also show that this distance is equivalent to the CP for single-qubit states.

The nonclassical distance D of a state ρ can be defined as the distance of ρ to the nearest state from the set of all classical states \mathcal{C} as [15, 18]:

$$D(\rho) = \frac{1}{2} \min_{\sigma \in \mathcal{C}} \mathcal{D}_{\mathrm{B}}^{2}(\rho, \sigma). \tag{22}$$

In this paper, and contrary to the original Refs. [15, 52], we assume the distance to be the Bures metric $D_{\rm B}(\rho,\sigma)$ [53], or equivalently the Helstrom metric [54], which is simply related to the fidelity $F(\rho,\sigma)$ as follows

$$\mathcal{D}_{\mathrm{B}}^{2}(\rho,\sigma) = 2[1 - \sqrt{F(\rho,\sigma)}]. \tag{23}$$

The fidelity is defined as [55]

$$F(\rho, \sigma) = \left(\text{Tr}\sqrt{\sqrt{\sigma}\rho\sqrt{\sigma}}\right)^2, \tag{24}$$

which can also be interpreted as a transition probability [56], or a quantum generalization of the Fisher information metric. Several methods for measuring or estimating the fidelity are known (see Ref. [57] and references therein). The fidelity for single-qubit states simplifies to

$$F(\rho, \sigma) = \text{Tr}(\rho\sigma) + \sqrt{(1 - \text{Tr}\rho^2)(1 - \text{Tr}\sigma^2)}.$$
 (25)

We mention that the Bures distance can be applied in quantifying not solely nonclassicality [18]. It has also found applications as indicators or measures of, e.g., state distinguishability [58], quantum entanglement [59, 60], quantum criticality [61], and light polarization [62].

It should be stressed that we look for the classical (or, least nonclassical) states, belonging to the Hilbert space of an investigated finite-dimensional system. Here we analyze the Hilbert space of a single qubit, defined as a superposition of the vacuum and single-photon Fock state. In this case the only classical state is the vacuum. Thus, we set $\sigma = |0\rangle\langle 0|$, then $F(\rho,|0\rangle) = \rho_{00} = 1 - p$. Thus, it is seen that such defined nonclassical distance is exactly equal to the CP,

$$D[\rho(p,x)] = CP[\rho(p,x)] = p, \tag{26}$$

for any values of $p \in [0,1]$ and $|x| \in [0,\sqrt{p(1-p)}]$. This correspondence provides another quantum information interpretation of the nonclassical distance.

We emphasize again that a nonclassical distance can be defined differently, both by choosing another distance measure and by extending the class \mathcal{C} of classical states, for which the minimization is performed. For example, in the original papers of Hillery [15, 52], the trace norm was used as a distance measure. While Dodonov *et al.* [16, 17, 20] applied the Hilbert-Schmidt distance. Moreover, the Kullback-Leibler distance [63], which is also known as information divergence, information gain, or relative entropy, can also be applied for quantifying nonclassicality, in analogy to the entanglement measures based on the relative entropy of entanglement [59, 64–68].

III. COMPARISON OF NONCLASSICALITY MEASURES

In general, for any single-qubit state $\rho=\rho(p,x)$, the following inequalities hold

$$\tau(\rho) \ge D(\rho) = \text{CP}(\rho) \ge \text{NP}(\rho).$$
 (27)

The left-hand inequality in Eq. (27) can be deduced by comparing explicitly the general expression for τ and D, given by Eqs. (8) and (26), respectively. The right-hand inequality in Eq. (27) is equivalent to the well-known inequality $C(\rho') \geq N(\rho')$ for the concurrence and negativity for arbitrary two-qubit states ρ' . Thus, in particular, for the states $\rho_{\rm out}$ generated by the BS from a single-qubit state ρ and the vacuum. Table I lists all four special cases of these inequalities, together with examples of states satisfying these cases.

In the following we analyze all the boundary states shown in Figs. 1 and 2, and discuss the relativity of nonclassical measures (see Tables II and III, and Fig. 3).

TABLE I: Examples of states satisfying all four special cases of the inequalities given in Eq. (27), where $\rho_0=\rho(\frac{1}{2},\frac{1}{4}),\, \rho_{\rm P}(p)\equiv\rho[p,\sqrt{p(1-p)}]$ is a pure state, and $\rho_{\rm M}(p)\equiv\rho(p,0)$ is a completely mixed state.

| Case | Nonclassicality measures | Examples of states ρ |
|------|-----------------------------------|---|
| 1 | $\tau(\rho) = D(\rho) = NP(\rho)$ | $ 0\rangle, 1\rangle$ |
| 2 | $\tau(\rho) > D(\rho) > NP(\rho)$ | $ ho_0$ |
| 3 | $\tau(\rho) > D(\rho) = NP(\rho)$ | $ \rho_{\mathrm{P}}(p) \text{ for } p \in (0,1) $ |
| 4 | $\tau(\rho) = D(\rho) > NP(\rho)$ | $ \rho_{\mathrm{M}}(p) \text{ for } p \in (0,1) $ |

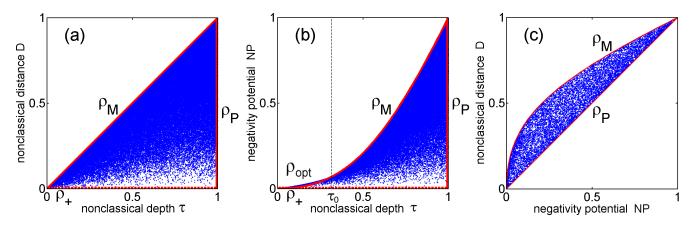


FIG. 1: (Color online) Allowed values of the nonclassicality measures for single-qubit states: (a) nonclassical distance D versus nonclassical depth τ , (b) negativity potential NP versus τ , and (c) D versus NP. The points correspond to a Monte Carlo simulation of 10^5 states ρ . Each point is plotted for $[D(\rho), \tau(\rho)]$ in (a) and analogously for panels (b) and (c). The vertical broken line in panel (b) is plotted at $\tau_0 \approx 0.3154$. The boundaries are given by pure states ρ_P [vertical red lines in the far right of (a) and (b), and the red diagonal line in (c)], completely mixed states ρ_M (solid red upper curves), as well as partially mixed states ρ_+ (bottom broken lines) and $\rho_{\rm opt}$ [corresponding to blue points right above the curve for ρ_M in (b)]. In (b), it is barely visible that ρ_M is not the upper bound for $\tau < \tau_0$. Thus, this region is magnified in Fig. 2(a). Note that, in a mathematical sense, there are no states corresponding exactly to the broken lines at the bottom of (a) and (b) for $0 < \tau \le 1$ and D = NP = 0. However, one can find states being arbitrarily close to these lines.

A. Boundary states

Figure 1 shows the nonclassicality regions for arbitrary single-qubit states. The points $[X(\rho),Y(\rho)]$ in these regions are obtained for the generated 10^5 states ρ by performing a Monte Carlo simulation. Here X and Y correspond to chosen nonclassicality measures. Thus, by analyzing these graphs in Fig. 1, one can say that some states are the most or least nonclassical in terms of a measure X for a given value of a measure Y.

Here we analyze the special cases of the general single-qubit state ρ , which correspond to the single-qubit boundary states shown in Figs. 1-3. We calculate the above-defined non-classicality measures for these states. In the Appendix, we present the proofs that they are indeed the boundary states.

1. Pure states

Equation (1) for $x=\sqrt{p(1-p)}$ reduces to a pure state $\rho_{\rm P}=|\psi_p\rangle\langle\psi_p|,$ where

$$|\psi_p\rangle = \sqrt{1-p}|0\rangle + \sqrt{p}|1\rangle.$$
 (28)

The BS output state for the input states $|\psi_p\rangle$ and $|0\rangle$, is simply given by

$$|\psi_{\text{out}}\rangle = \sqrt{1-p}|00\rangle + \sqrt{\frac{p}{2}}(|10\rangle - i|01\rangle).$$
 (29)

By recalling that

$$C(|\psi_{\text{out}}\rangle) = N(|\psi_{\text{out}}\rangle) = 2|c_{00}c_{11} - c_{01}c_{10}|$$
 (30)

for a general two-qubit pure state $|\psi\rangle=\sum_{m,n=0,1}c_{mn}|mn\rangle$, where c_{mn} are the normalized complex amplitudes, one can

obtain the nonclassical measures as follows

$$NP(|\psi_p\rangle) = D(|\psi_p\rangle) = \rho_{11} = p. \tag{31}$$

By contrast to these equal measures, the nonclassical depth for a pure state reads

$$\tau(|\psi_p\rangle) = 1 - \delta_{p,0},\tag{32}$$

in terms the Kronecker delta $\delta_{p,0}$. In the special cases of the vacuum and single-photon states, this formula reduces to the known results [24]. It is clearly seen that the depth τ is discontinuous, as $\tau[|\psi(p=1)\rangle] \equiv \tau(|0\rangle) = 0$, while $\tau[|\psi(p>0)\rangle] = 1$, even for p very close to zero. Note that also the entanglement potential based on the Schmidt number is discontinuous.

Pure states are the boundary states in the three panels of Fig. 1 for the whole range [0,1] of the ordinate. In particular, they correspond to the lower bound of the nonclassical distance versus NP. Note that we are analyzing the potential based on the negativity rather than the logarithmic negativity, as suggested and applied in Ref. [38]. Thus, the lower bound in Fig. 1(c) is given by a straight line, which would not be the case otherwise.

2. Completely mixed states

In another special case, Eq. (1) for x=0 describes a completely mixed state,

$$\rho_{\mathcal{M}} = (1 - p)|0\rangle\langle 0| + p|1\rangle\langle 1|,\tag{33}$$

i.e., a statistical mixture of the vacuum $|0\rangle$ and single-photon state $|1\rangle.$ Thus, we have

$$\tau(\rho_{\mathcal{M}}) = D(\rho_{\mathcal{M}}) = p. \tag{34}$$

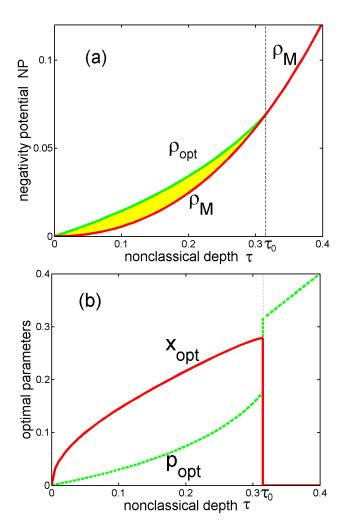


FIG. 2: (Color online) (a) The inset of Fig. 1(b) showing, in greater detail, the boundaries for the NP versus nonclassical depth τ . These boundaries are reached by the partially mixed optimal states $\rho_{\rm opt}$ for $\tau < \tau_0$ and completely mixed states $\rho_{\rm M}$ for $\tau \geq \tau_0$. For clarity, we do not plot here points corresponding to our Monte Carlo simulation shown in Fig. 1. (b) Optimal parameters $p_{\rm opt} = \langle 1|\rho_{\rm opt}|1\rangle$ and $x_{\rm opt} = |\langle 0|\rho_{\rm opt}|1\rangle|$ as a function of τ . These parameters are discontinuous at $\tau = \tau_0$, but, for clarity, we have plotted the red and green vertical connecting lines at this point.

The NP for any mixed state $\rho_{\rm M}(p)$ can be found from the general formula given in Eq. (14), but here we apply a more explicit and intuitive derivation. Specifically, if the input qubit state is completely mixed, then one finds that the BS output state reads

$$\rho_{\text{out}}(p,0) = U_{\text{BS}}[\rho_{\text{M}}(p) \otimes |0\rangle\langle 0|]U_{\text{BS}}^{\dagger}
= p|\bar{\psi}^{-}\rangle\langle\bar{\psi}^{-}| + (1-p)|00\rangle\langle 00|, \quad (35)$$

where $|\bar{\psi}^-\rangle = (|10\rangle - i|01\rangle)/\sqrt{2}$. This is the statistical mixture of a maximally entangled state and a separable state orthogonal to it, which is often referred to as the Horodecki state [8]. Such mixtures are often studied in the comparisons of various entanglement and nonlocality measures [65, 67–

70]. Thus, the NP for a mixed $\rho_{\rm M}(p)$ reads as

$$NP(\rho_M) = N[\rho_{out}(p,0)] = \sqrt{(1-p)^2 + p^2} - (1-p).$$
 (36)

Completely mixed states are the boundary states shown in the three panels of Fig. 1. However, it is worth noting that they are *not* extremal for the whole range of τ in Fig. 1(b), which is shown in detail in Fig. 2(a) and discussed in the next paragraph.

3. Partially mixed optimal states

A preliminary analysis of Fig. 1(b) can lead to a conjecture that: completely mixed states ρ_M correspond to the upper boundary of the NP for an arbitrary value of the depth $\tau \in [0,1]$. However, a closer scrutiny of Fig. 2(a), which is the inset of Fig. 1(b), indicates that ρ_M is the extremal state only for $\tau \geq \tau_0$. This critical value is $\tau_0 \approx 0.3154$, as marked by the vertical broken lines in Figs. 1(b) and 2. By contrast to this, there are other states exhibiting higher nonclassicality if $\tau < \tau_0$. Thus, let us define the following partially mixed state

$$\rho_{\text{opt}}(\tau) \equiv \rho[p_{\text{opt}}(\tau), x_{\text{opt}}(\tau)],$$
(37)

where $x_{\rm opt}^2(\tau)=p_{\rm opt}(\tau)-p_{\rm opt}^2(\tau)/ au$, which corresponds to the maximum NP for a given au [as shown in Fig. 2(a)], i.e.,

$$NP(\rho_{\text{opt}}(\tau)) \equiv \max_{p} NP[\rho(p, \sqrt{p - p^2 \tau^{-1}})]. \tag{38}$$

The optimal matrix elements $p_{\rm opt}$ and $x_{\rm opt}$ are shown as a function of τ in Fig. 2(b). These elements can easily be obtained by numerically maximizing Eq. (14), with $|x|^2 = p - p^2/\tau$, for a given τ . It is seen that $p_{\rm opt} = \tau$ and $x_{\rm opt} = 0$ for $\tau \geq \tau_0$, thus $\rho_{\rm opt}$ becomes ρ_M in this range of τ . Unfortunately, we have not found a compact-form analytical expression for $\rho_{\rm opt}$ for $\tau < \tau_0$.

4. Partially mixed states with nonzero τ for vanishing D and NP

We also analyze the state $\rho(p,x)$ defined in the right-hand limit $p\to 0+$ with properly chosen x as follows:

$$\rho_{+}(\tau_{0}) = \lim_{p \to 0+} \rho(p, x_{0}), \tag{39}$$

where

$$x_0 = \sqrt{(1+p-\tau_0^{-1}p)p(1-p)},$$
 (40)

assuming $\tau_0 \in (0,1]$. Note that pure states with $\tau_0 = 1$ can also be considered here. To be more explicit, let us analyze the special case of $\rho(p,x_0)$, when $\tau_0 = 1/2$ and

$$p = D[\rho(p, x_0)] = 10^{-n} \Rightarrow \tau[\rho(p, x_0)] = \frac{1}{2 - 10^{-n}},$$
 (41)

for $n=0,1,2,\ldots<\infty$. It is seen that the nonclassical depth is approaching the chosen nonzero value $\tau_0=1/2$ at the same

rate as the nonclassical distance is vanishing. In general, we can write:

$$\tau[\rho_{+}(\tau_{0})] \equiv \lim_{p \to 0+} \tau[\rho(p, x_{0})] = \tau_{0},$$

$$NP[\rho_{+}(\tau_{0})] \equiv \lim_{p \to 0+} NP[\rho(p, x_{0})] = 0,$$

$$D[\rho_{+}(\tau_{0})] \equiv \lim_{p \to 0+} D[\rho(p, x_{0})] = 0.$$
(42)

Thus, this state approaches the lower bound of the distance D versus depth τ [shown as the bottom broken line in Fig. 1(a)] and the NP versus depth τ [see bottom of Fig. 1(b)]. Because of the discontinuity of the depth τ , these lower bounds in Figs. 1(a) and 1(b) are not exactly reached, as indicated by the broken lines. This is also reflected in the definition of ρ_+ given by the right-hand limit in Eq. (39). Thus, strictly speaking NP(ρ) = 0 (or, equivalently, $D(\rho)$ = 0) for a given state ρ if and only if $\tau(\rho)$ = 0. This is because all these quantities are measures (rather than only witnesses) of nonclassicality, and thus they give the necessary and sufficient conditions for the nonclassicality of an arbitrary single-qubit state ρ .

B. Mixtures of states can be more nonclassical than their superpositions

The analysis of Fig. 1 can lead to the conclusion that the completely mixed states $\rho_{\rm M}$ are the most nonclassical single-qubit states with respect to: (i) the distance D for a given value of the depth $\tau \in [0,1]$, (ii) D for a fixed value of the NP $\in [0,1]$, and (iii) the NP for a given value of $\tau \in [\tau_0,1]$. Conversely, pure states $\rho_{\rm P}$ are the most nonclassical single-qubit states regarding τ versus D, τ versus NP, and NP versus D.

This interpretation of the maximum nonclassicality of mixed states should not be confused with the following conclusion that dephasing could increase the nonclassicality. Such dephasing results in decreasing the off-diagonal term x, while keeping the diagonal terms unchanged. Specifically, one can observe that

$$\tau[\rho_{P}(p)] \geq \tau[\rho(p,x)] \geq \tau[\rho_{M}(p)],$$

$$NP[\rho_{P}(p)] \geq NP[\rho(p,x)] \geq NP[\rho_{M}(p)],$$

$$D[\rho_{P}(p)] = D[\rho(p,x)] = D[\rho_{M}(p)],$$
(43)

for any $x \in [0,1]$. It is seen that by decreasing x, also $\tau[\rho(p,x)]$ and $\mathrm{NP}[\rho(p,x)]$ decrease, while only $D[\rho(p,x)]$ remains unchanged. Thus, in this interpretation based on the inequalities in Eq. (43), a mixed state $\rho_{\mathrm{M}}(p)$ is not more nonclassical than a pure state $\rho_{\mathrm{P}}(p)$ assuming the same element p.

C. Relativity of nonclassicality measures

The nonclassicality measures can give different predictions not only concerning the absolute values, but more importantly, Our reverse conclusion about *mixed states*, which are more nonclassical than superposition states (including pure states), refers to another comparison. To show this more explicitly, we express $\rho(p,x)$ in terms of some nonclassicality measures instead of the parameters p,x. In particular, by inverting Eq. (8) for $\tau=\tau[\rho(p,x)]$ and by applying $D=D[\rho(p,x)]=p$, one can express a general single-qubit state (assuming real x) in terms of these nonclassicality measures, i.e.,

$$\rho(p,x) \equiv \rho'(D,\tau) = \begin{bmatrix} 1 - D & \sqrt{D - D^2 \tau^{-1}} \\ \sqrt{D - D^2 \tau^{-1}} & D \end{bmatrix},$$
(44)

where $\tau \in [0,1]$ and $D \in [0,\tau]$. Analogously, we can express $\rho(p,x)$ in terms of other pairs of nonclassicality measures, e.g.,

$$\rho(p,x) \equiv \rho''(N,\tau) = \rho'''(N,D),\tag{45}$$

where $N=\mathrm{NP}[\rho(p,x)]$, although the expressions will be much more complicated here. Analogously, we introduce the symbols ρ_{M}' , ρ_{M}'' , and ρ_{M}'' , denoting the mixed state ρ_{M} , which is expressed via the nonclassical measures analogously to ρ' , ρ'' , and ρ''' , respectively. Note that the assumption of real x follows from the property that the nonclassical measures τ and NP depend solely on the absolute value of x, while D is completely independent of x.

Thus, for a given value of the nonclassical depth, say $\tau_1 \in [0,1]$, one can observe that

$$D[\rho'_{\mathcal{M}}(D_1, \tau_1)] \ge D[\rho'(D', \tau_1)],$$
 (46)

where $D' \in [0, \tau_1]$ and $D_1 = \tau_1$. For a given value of the depth $\tau_1 \in [\tau_0, 1]$, where $\tau_0 = 0.3154$, one finds that

$$NP[\rho''_{M}(N_{1}, \tau_{1})] \ge NP[\rho''(N'', \tau_{1})],$$
 (47)

where $N'' \in [N_0, N_1]$ and $N_i = \sqrt{(1-\tau_i)^2 + \tau_i^2} - (1-\tau_i)$ for i=0,1. Moreover, for a given value of the NP, say $N_1 \in [0,1]$, one observes that

$$D[\rho_{\mathcal{M}}^{\prime\prime\prime}(D_1, N_1)] \ge D[\rho^{\prime\prime\prime}(D^{\prime\prime\prime}, N_1)],\tag{48}$$

where $D''' \in [N_1,1]$ and here $D_1 = \sqrt{2N_1(1+N_1)} - N_1$. All these three inequalities show that completely mixed states can be considered as the most nonclassical single-qubit states for a fixed value of a proper nonclassical measure, as shown in the corresponding panels of Fig. 1.

regarding the ordering of states. In other words, by comparing two states we cannot usually judge which of them is more nonclassical.

It is somehow surprising that any pure state (different from

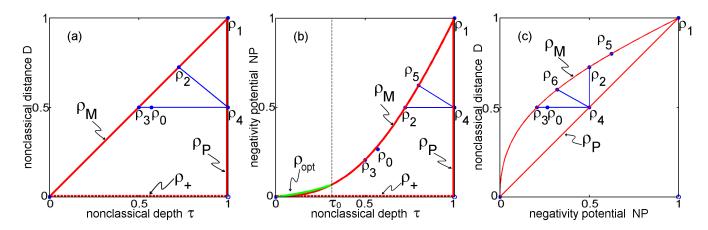


FIG. 3: (Color online) Particular single-qubit states ρ_n defined explicitly in Table II and plotted in analogy to Fig. 1. As in Fig. 1, here the boundaries are given by pure states ρ_P , completely mixed states ρ_M , together with the partially mixed states ρ_+ and $\rho_{\rm opt}$. There are no states corresponding exactly to the broken lines and empty circles. Any inequality listed in Table III can be satisfied by properly choosing pairs of these states. This analysis demonstrates the *relativity of nonclassicality measures*.

TABLE II: Definition of states ρ_n , also shown in Fig. 3, and the analytical values of their four nonclassicality measures. These states are chosen for discussion of the relativity of the nonclassicality ordering of general states.

| state ρ_n | $\tau(\rho)$ | $D(\rho) = \mathrm{CP}(\rho)$ | $NP(\rho)$ |
|---|---------------------------|-------------------------------|--|
| $\rho_0 = \rho(\frac{1}{2}, \frac{1}{4})$ | $\frac{4}{7}$ | $\frac{1}{2}$ | $\cos(\tfrac{2}{9}\pi) - \tfrac{1}{2}$ |
| $\rho_1 = 1\rangle\langle 1 $ | 1 | 1 | 1 |
| $ \rho_2 = \rho_{\rm M} [\frac{1}{2} (\sqrt{6} - 1)], $ | $\frac{1}{2}(\sqrt{6}-1)$ | $\frac{1}{2}(\sqrt{6}-1)$ | $\frac{1}{2}$ |
| $ \rho_3 = \rho_{\mathrm{M}}(\frac{1}{2}) $ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}(\sqrt{2}-1)$ |
| $\rho_4 = \rho_{\rm P}(\frac{1}{2})$ | 1 | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $ \rho_5 = \rho_{\mathrm{M}}(\frac{4}{5}) $ | $\frac{4}{5}$ | $\frac{4}{5}$ | $\frac{1}{5}\left(\sqrt{17}-1\right)$ |
| $\rho_6 = \rho_{\rm M}(\frac{3}{5})$ | $\frac{3}{5}$ | $\frac{3}{5}$ | $\frac{1}{5}\left(\sqrt{13}-2\right)$ |

the vacuum) has the same maximum nonclassicality with respect to the nonclassical depth, which is not the case for the other discussed measures.

A natural conjecture concerning basic properties of good nonclassicality measures can be formulated as follows: By comparing the values of such measures for a pair of arbitrary states ρ' and ρ'' , one can order them uniquely. Specifically, they should have the same degree of nonclassicality or one of them should be less nonclassical than the other according to all good nonclassicality measures. For example, if $\tau(\rho') < \tau(\rho'')$, then the same inequality should also hold for other measures including the NP and D. However, one can falsify this conjecture by recalling a deeper relation between some nonclassicality and entanglement measures and by referring to the works, where the relativity of entanglement measures has already been demonstrated [65, 69, 71-73]. Here detailed comparisons, shown in Table III and Fig. 3, give evidence for this relativity even for nonclassicality measures, which are not directly related to entanglement.

TABLE III: Inequalities and examples of pairs of states (ρ_n, ρ_m) satisfying them. The states ρ_n (with $n=1,\ldots,6$) are defined in Table II and are plotted in Fig. 3. Some inequalities imply same orderings, and others involve different orderings of single-qubit states by the nonclassical measures: depth τ , distance D, and negativity potential NP.

| 1 | $\tau(\rho_1) > \tau(\rho_2)$ | and | $D(\rho_1) > D(\rho_2)$ |
|----|-------------------------------|-----|---------------------------|
| 2 | $	au(ho_1) = 	au(ho_4)$ | and | $D(\rho_1) > D(\rho_4)$ |
| 3 | $	au(ho_4) > 	au(ho_3)$ | and | $D(\rho_4) = D(\rho_3)$ |
| 4 | $\tau(\rho_2) < \tau(\rho_4)$ | and | $D(\rho_2) > D(\rho_4)$ |
| | | | |
| 5 | $	au(ho_1) > 	au(ho_2)$ | and | $NP(\rho_1) > NP(\rho_2)$ |
| 6 | $\tau(\rho_1) = \tau(\rho_4)$ | and | $NP(\rho_1) > NP(\rho_4)$ |
| 7 | $	au(ho_4) > 	au(ho_2)$ | and | $NP(\rho_4) = NP(\rho_2)$ |
| 8 | $	au(ho_5) < 	au(ho_4)$ | and | $NP(\rho_5) > NP(\rho_4)$ |
| | | | |
| 9 | $NP(\rho_1) > NP(\rho_2)$ | and | $D(\rho_1) > D(\rho_2)$ |
| 10 | $NP(\rho_2) = NP(\rho_4)$ | and | $D(\rho_2) > D(\rho_4)$ |
| 11 | $NP(\rho_4) > NP(\rho_3)$ | and | $D(\rho_4) = D(\rho_3)$ |
| 12 | $NP(\rho_6) < NP(\rho_4)$ | and | $D(\rho_6) > D(\rho_4)$ |

IV. CONCLUSIONS

Various measures of the amount of nonclassicality have been proposed with respect to the definition of nonclassicality based on the nonpositivity of the P function. Here we have applied the following measures to quantify the nonclassicality of single-qubit states: the Lee nonclassical depth τ , the Hillery nonclassicality distance D, and the entanglement potentials NP and CP.

We have found analytical expressions for these measures for the simplest nontrivial example of single-qubit photonnumber states. These formulas clearly show the relativity of ordering states with nonclassicality measures, as summarized in Tables I and III. Only the CP and nonclassical distance were found to be equivalent.

Further, we have found maximally and minimally nonclassical states by comparing any two of these measures. Surprisingly, statistical mixtures of states can be more nonclassical than their superpositions. Indeed, mixed states are the most nonclassical if one considers the nonclassicality distance for a given value of either the nonclassical depth or of the NP in the whole range [0,1] of the abscissa, as well as the NP versus the nonclassical depth τ such that $\tau \geq \tau_0$, where $\tau_0 = 0.3154\ldots$, as shown in Fig. 1. However, there are partially mixed states, which have the NP for a given value of $\tau \in [0,\tau_0)$ slightly larger than for completely mixed states, as shown in Figs. 1(b) and 2(a).

Both of our results, concerning (i) the relativity of ordering states with nonclassicality measures and (ii) the nonclassicality of mixed states exceeding that of superposition states, are a consequence of the nonequivalence of some of the most popular measures of nonclassicality, including the nonclassical depth, nonclassical distance, and NP. There are also equivalent measures, including the nonclassical distance, CP, and the potential for the entanglement of formation, as given by Eq. (20). Clearly, the above mentioned counterintuitive properties do not appear for such equivalent measures.

We found that the nonclassical distance D, as defined for the specific choice of the reference classical states, corresponds to the CP for arbitrary single-qubit states. This result shows an operational interpretation of this nonclassical distance as the potential for the entanglement of formation.

The present analysis can be extended to similar comparative studies of other quantitative measures of nonclassicality of single-, two-, and multimode systems. In particular, one can focus on the comparative approaches to quantify the nonclassicality of correlations as listed in, e.g., Ref. [74].

We believe that our study could further stimulate interest in the nonclassicality measures applied to finite-dimensional systems in finding their general properties including their operational interpretations.

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Appendix A: Proofs for boundary states

Here we prove that completely mixed states $\rho_{\rm M}$, pure states $\rho_{\rm P}$, and partially mixed states, $\rho_{\rm opt}$ and ρ_{+} , are the boundary (or extremal) states shown in Figs. 1 and 2. Specifically:

- (1) The upper bound in Fig. 1(a): As $\tau(\rho) \geq D(\rho)$ holds for any single-qubit ρ as given in Eq. (27), then it is seen that this bound is reached by the completely mixed states $\rho_{\rm M}$, for which it holds $\tau(\rho_{\rm M}) = D(\rho_{\rm M})$.
- (2) The upper bound in Figs. 1(b) and Fig. 2(a) was obtained numerically by maximizing a single-variable function of the NP, given in Eq. (14) with $|x|^2 = p p^2/\tau$, for a given τ . In particular, the completely mixed states $\rho_{\rm M}$ correspond to this upper bound for $\tau > \tau_0$. Indeed, $\rho_{\rm M}$ satisfy the Karush-Kuhn-Tucker (KKT) conditions, as can be shown analogously to the method applied for the two-qubit measures of entanglement and Bell nonlocality [67, 68, 70]. We note that these KKT conditions correspond to a refined method of Lagrange multipliers [75].
- (3) The upper and lower bounds in Fig. 1(c): The area in the relation between the nonclassical distance (or, equivalently, CP) and NP of *arbitrary single-qubit* states is the same as the area in the relation between the concurrence and negativity of *arbitrary two-qubit* states. As shown in Ref. [76], the two-qubit pure states and the Horodecki states are the extremal states for the concurrence versus negativity, but these states can be generated from the pure and mixed single-qubit states, respectively, as discussed in Sec. III.A. Thus, the pure and mixed single-qubit states are the extremal states for the relation between the nonclassical distance and NP.
- (4) The lower and right-hand bounds in Figs. 1(a) and 1(b) are implied from the property that all these measures have their values in the range [0, 1].

This concludes our proofs of the boundary states.

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